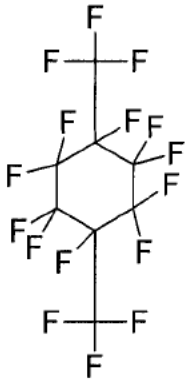
STRUCTURE ACTIVITY TEAM REPORT ver. 04/98	[redacted]
Case #: L-07-0368	**DCN:**
SAT Date: 8/28/2007	**SAT Chair:** L. Keifer
Submitter: Tracerco	

Chemical Name:

Cyclohexane, 1,1,2,2,3,4,4,5,5,6-decafluoro-3,6-bis(trifluoromethyl)-

CAS RN:	Trade Name:
374-77-6	FLUTEC TG n-PDMCH, Tracerco 400c

Structure



[redacted]

Molecular Formula:	C_8F_{16}		
Molecular Wt. 400	**WT%<500:**	**WT%<1000:**	
MP:	**BP:**	**Eq. Wt:**	
H2O Sol (g/L): <0.000001	**V.P.** 36.0000		
Max. Prod. Volume (kg/yr): 300	**Physical State:** Liquid		

USE:

Tracer chemical for measuring flow of gas in deep oil/gas bearing geological strata
STN file CA 35 references found
P2REC CRSS. Forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata.

Related Case Numbers	Case Role	Related Case Numbers	Case Role
[redacted]		[redacted]	

Focus Date: 9-13-07 Results: Final Cond Grant

STRUCTURE ACTIVITY TEAM REPORT [redacted] 08/28/07

CASE NUMBER: **L07-0368**

RELATED CASES: [redacted] [redacted] [redacted]

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL OF CONCERN:	1-2	1

KEYWORDS: NEURO CARDIAC SENS (UNCERT)

SUMMARY OF ASSESSMENT

FATE: Liquid with MP < 20 °C (E)
log Kow = 4.75 (E);
S = 0.343 mg/L at 25 °C (E)
VP = 36 torr at 25 °C (M)
BP = 101.7 °C (M)
H = 5.66E+4 (E)
log Koc = 5.94 (E)
log Fish BCF = 2.96 (E)
POTW removal (%) ≥ 99 via sorption and stripping
Time for complete ultimate aerobic biodeg > mo
Sorption to soils/sediments = v.strong
Volatilization half-life from a standard river = 2 hrs
Volatilization half-life from a standard lake = 8 da
PBT Potential: P3B1T1
*CEB FATE: Migration to ground water = negl

HEALTH: Expect poor absorption via all routes (pchem). In the Standard Review for the analogue [redacted] neurotoxicity was the only effect supported. Uncertain concern for cardiac sensitization.

*CEB HEALTH: Low moderate concern (Dermal, inhalation)

P2 DISCUSSION: SAT judged that replacing radioactive materials with inert materials in the work place is a good idea.

*CCD P2 RECOGNITION: RECOMMENDED

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=	*	P
daphnid 48-h LC50	=	*	P
green algal 96-h EC50	=	*	P
fish chronic value	=	*	P
daphnid ChV	=	*	P
algal ChV	=	*	P

Predictions are based on SARs for neutral organic chemicals; SAR chemical class = alkane-C8-cyclic-perF; MW400; liquid with mp = -16 C (P); log Kow = 7.5 (ACD); S < 0.001 mg/L at 20 C (P); pH7; effective concentrations based on 100% active ingredients, closed vessel with no head space, and mean measured concentrations; hardness <150.0 mg/L as CaCO3; and TOC <2.0 mg/L;
low concern for toxicity;
assessment factor = 10.0
concern concentration = *
*CEB ECOTOX: No releases to water

SAT Co-chair: Leonard Keifer 564-8916

NCSAB SAT REPORT [redacted]

PMN:	L-07-0368	CAS RN:	374-77-6

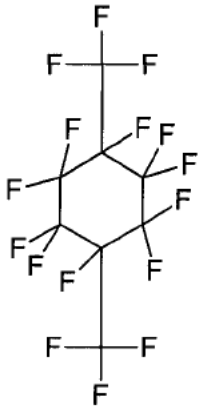
Chemical Name:

Cyclohexane, 1,1,2,2,3,4,4,5,5,6-decafluoro-3,6-bis(trifluoromethyl)-

Analogs:

Production Volume: 300.00

Structure:



Use:
Tracer chemical for measuring flow of gas in deep oil/gas bearing geological strata.
STN file CA: 35 references found.
P2REC: CRSS: Forward. P2 Claim: The LVE substance is a substitute for radionuclide tracers to measure the flow rate in oil-bearing strata.

Formula:	C_8F_{16}	Eq Wt:		
Mol Weight:	400.06	Wt%<500:		Wt%<1000
MP:		BP:	101.70	VP:
H2O Sol (g/L):	<0.000001	Physical State:	Liquid	Log P: 7.5 (ACD)

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	*		
Daphnid 48-h	*		
Algal 96-h	*		
Fish ChV	*		
Daphnid ChV	*		
Algal ChV	*		
BCF			

CHEMICAL CLASS: SAR: cyclic alkane - C8 - per F

ECOTOX CONCERN: H | M | (L) CONCERN CONCENTRATION: *

DATE 8/28/07 ASSESSOR:

GTOX Report

PMN No. [redacted] CAS No. [redacted] Rcvd: 07/20/98 OECD Incomplet ID: Rec# 0 : 1423

S/A Name of Analog

Reviewer OEO

		with activation	without activation	Positive Strains
Salmonella Assay:		☐	☐	
Chromosomal Aberration	CHO:	☐	☐	
	CHL:	☐	☐	
	V79:	☐	☐	
E. coli Reverse Mutation:		☐	☐	
Mouse Micronucleus Assay:	Route:		☐	
Rat Hepatocytes Unscheduled DNA Synthesis:			☐	

Other GTOX Results

Comments

ECOTOX: ☐

Fate: BOD/COD of [redacted], page 83.

WS/Log P:

Toxicology Report

PMN No. [redacted] CAS No. [redacted] Rcvd: 07/20/98 OECD Incomplete ID: Rec# 0 : 1423

S/A: S | Name of Analog: | Reviewer: OEO | Study#: 2351

Study Type	Species	Sex	Route
Acute Toxicity	Rat	MF	Oral (unspec)

Test Substance Description

Test substance administered as supplied.

Test Conditions

Duration: 14 days; Wt: 91-128 g; Groups: 2/10; Controls: ; Dose: 100 ml/kg bodyweight; Test Conditions: Single oral dose over a six hour period.

Results

No mortalities, clinical signs of toxicity, or abnormalities at necropsy was observed.

Toxicology Report

PMN No. [redacted] CAS No. [redacted] Rcvd: 07/20/98 OECD: Incomplete ID: Rec# 0 : 1423

S/A: S Name of Analog: Reviewer: OEO Study#: 2352

Study Type: Acute Toxicity Species: Rat Sex: NS Route: Inhalation

Test Substance Description

Vapor

Test Conditions

Duration: 14 days; Wt: NS; Groups: 1/10; Controls: ; Dose: 4% v/v [redacted] vapor; Test Conditions: Continuous exposure to test substance for six hours

Results

There were no signs of irritation during exposure and during a 14 day post exposure observation period. Apart from a transient weight loss in the male rats, the performance of the test group of animals was comparable with that of the control group. No abnormalities were observed at necropsy. It was concluded that the samples of [redacted] have no appreciable acute inhalation toxicity to rat.

Toxicology Report

PMN No. [redacted] CAS No. [redacted] Rcvd: 07/20/98 OECD: Incomplete ID: Rec# 0 : 1423

S/A: S Name of Analog: Reviewer: OEO Study#: 2353

Study Type: Eye Irritation Species: Rabbit Sex: NS Route: Eyes

Test Substance Description

Clear, colorless liquid dosed as received.

Test Conditions

Duration: 72 hours; Wt: young adults/2214-2441 g; Groups: 1/3; Controls: ; Dose: 0.1 ml; Test Conditions: Instillation on the everted lower lid of one eye, with the contralateral eye serving as the untreated control.

Results

No signs of corneal or iridial irritation or toxicity was noted.

Toxicology Report

PMN No. [redacted] CAS No. [redacted] Rcvd: 07/20/98 OECD Incomplete ID: Rec# 0 : 1423

S/A: S | Name of Analog: | Reviewer: OEO | Study#: 2354

Study Type	Species	Sex	Route
Dermal Irritation	Rabbit	NS	Dermal

Test Substance Description

Clear colorless liquid.

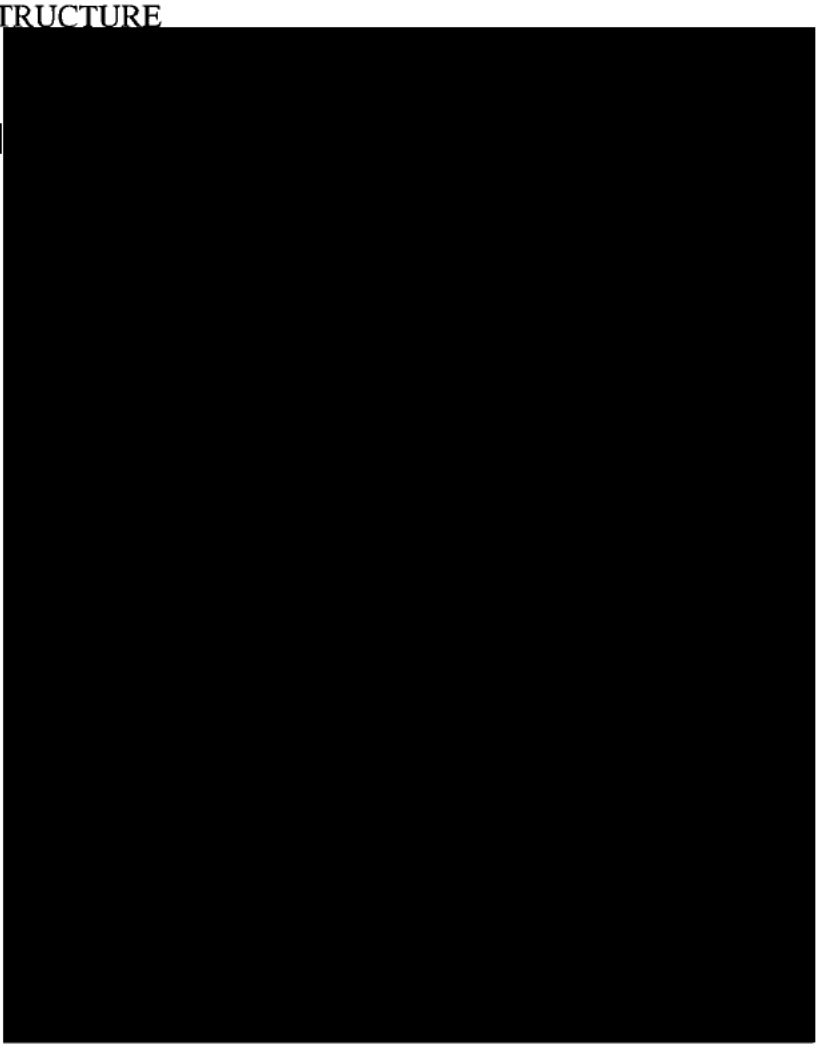
Test Conditions

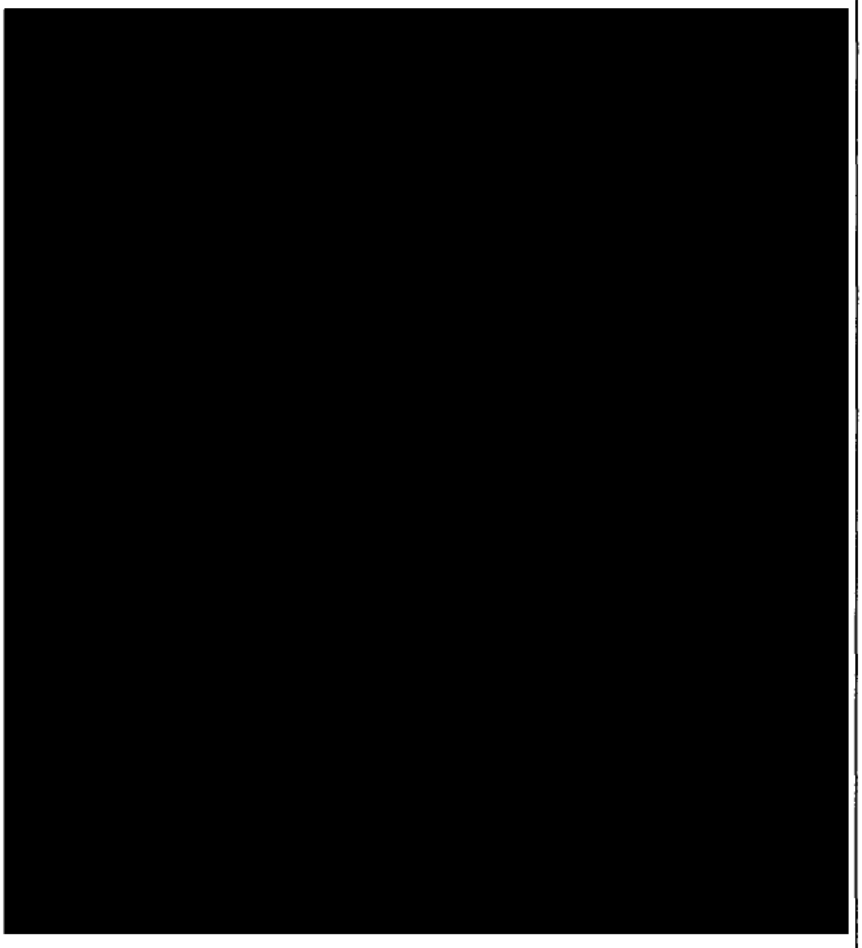
Duration: 7 days; Wt: 2246- 2359g/ young adults; Groups: 1/3; Controls: ; Dose: 0.5 ml; Test Conditions: 4 -hour single application to intact site.

Results

No dermal irritation was observed in any animal during the study period.

L07-368

ID [redacted]	STRUCTURE 
CAS [redacted]	
MOL WEIGHT [redacted]	
POINTER PMN	
MOL FORMULA [redacted]	
SAT HEALTH 1-2	
SAT ECO 2	
DISPO STANDARD REVIEW-HEALTH,FATE EXPOSURE-BASED-HEALTH,FATE	KWD AQUATOX-A,C GLOBAL-WARMING SENS-CARDIO SOLVENT-NEURO
COMMENTS	
NAME [redacted]	

ID [redacted]	STRUCTURE 
CAS [redacted]	
MOL WEIGHT [redacted]	
POINTER LOW VOLUME	
MOL FORMULA [redacted]	
SAT HEALTH 1	
SAT ECO 3	
DISPO CONDITIONAL GRANT	KWD AQUATOX-A,C GLOBAL WARMING
COMMENTS	
NAME [redacted]	

ID	STRUCTURE
[redacted]	[redacted]
CAS [redacted]	
MOL WEIGHT [redacted]	
POINTER LOW VOLUME	
MOL FORMULA [redacted]	
SAT HEALTH 1	
SAT ECO 3	
DISPO GRANTED/REFER TO OAR FOR GLOBAL WARMING ISSUES	KWD AQUATOX-C
COMMENTS	
NAME [redacted]	

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 8-28-07

ATTENDEES	SIGNATURE
CHEMISTRY	
✓ Paul Bickart	Paul Bickart
___ Diana Darling	
___ Rich Engler	
___ Greg Fritz	
___ Daniel Lin	
✓ Kathy Schechter	Kathy Schechter
___ _____	
ENVIRONMENTAL FATE	
___ Bob Boethling	
___ Wen-Hsiung Lee	
✓ Laurence Libelo	
___ David Lynch	
___ Andy Mamantov	
___ _____	
HEALTH	
___ Katherine Anitole	
✓ Michael Cimino	
___ Steve Cragg	
___ Leonard Keifer	
___ David Lai	
✓ Jim Murphy	
___ Deborah Norris	
✓ Ronald Ward	
✓ Yin Tak Woo	
___ _____	
___ _____	
ENVIRONMENTAL EFFECTS	
✓ Gordon Cash	MEMO
✓ Vince Nabholz	
___ Maggie Wilson	
___ _____	
SAT CHAIR/OTHER	
___ Rebecca Jones	
✓ Leonard Keifer	
___ Vince Nabholz	
✓ Jim Kwiat	
___ _____	